

Table S1 Configuration of WRF-NAQPMS-APM

Configuration	Description
Horizontal resolution	27 km, 9 km
Vertical layers	30
Microphysics	Lin (Lin et al., 1983)
Short-wave radiation	Goddard (Chou and Suarez, 1994)
Long-wave radiation	Goddard (Mlawer et al., 1997)
Land-surface	Noah (Chen and Dudhia, 2001).
Boundary layer	YSU (Hong et al., 2006)
Cumulus	New Grell
Anthropogenic emission	MEIC (Li et al., 2017)
Gas chemistry	CBMZ (Zaveri and Peters, 1999)
SOA	VBS (Yang et al., 2019)
Heterogeneous chemistry	Li et al., 2018
Microphysics	APM (Chen et al., 2014)
Dry deposition	Wesely

Table S2 List of physical and chemical properties of species concerned in FlexAOD

Species	Density (g/cm ³)	Refractive index @550nm	Mean radius (μm)	Standard deviation	Growth factor at RH=80%
Sulfate	1.77	1.53-0.06i	0.05	2	1.64
Nitrate	1.73	1.53-0.06i	0.065	2	1.64
Secondary organic	1.3	1.43	0.095	1.5	1.64
Primary organic	1.47	1.63-0.021i	0.12	1.3	1
BC	1.8	1.85-0.71i	0.03	1.8	1
PPM	2.65	1.56-0.014i	0.31	1.5	1
Fine dust	2.5	1.56-0.014i	1.9	2.2	1

Table S3 Formula of statistic parameters used in this study

Statistical parameter	Calculation formula
R (Correlation Coefficient)	$R = \frac{\{\sum_{i=1}^N (M_i - MM)(O_i - MO)\}}{\{\sum_{i=1}^N (M_i - MM)^2 (O_i - MO)^2\}^{\frac{1}{2}}}$
FAC2 (Fraction of data that satisfy $0.5 \leq \frac{M_i}{O_i} \leq 2$)	FAC2= NV/N
NMB (Normalized Mean Bias)	$NMB = \left[\sum_{i=1}^N M_i - O_i \right] / \sum_{i=1}^N O_i$
MFB (Mean Fractional Bias)	$MFB = \frac{1}{N} \sum_{i=1}^N \frac{(M_i - O_i)}{[(M_i + O_i)/2]}$
MFE (Mean Fractional Error)	$MFE = \frac{1}{N} \sum_{i=1}^N \frac{ M_i - O_i }{[(M_i + O_i)/2]}$

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Table S4 Statistic parameters between observed and simulated PM_{2.5}

Parameter	Beijing	Tangshan	Tianjin	Baoding	Hengshui	Zhengzhou	Benchmark
R	0.75	0.69	0.76	0.65	0.70	0.55	>0.40 ^a
NMB	-0.01	-0.09	-0.18	-0.22	-0.14	0.13	≤ ± 0.3 ^a
PM _{2.5} IOA	0.85	0.83	0.85	0.72	0.80	0.72	
MFB	0.12	-0.18	-0.21	-0.17	-0.13	0.15	≤ ± 0.6 ^b
MFE	0.50	0.44	0.41	0.44	0.32	0.41	≤ ± 0.75 ^b

^a Emery et al., 2016

^b Boylan and Russell. 2006

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